Spin-liquid versus dimerized ground states in a frustrated Heisenberg antiferromagnet

Luca Capriotti,[1] Douglas J. Scalapino,[2] and Steven R. White[3]
[1] *Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106-4030*
[2] *Department of Physics, University of California, Santa Barbara, California 93106-9530*
[3] *Department of Physics and Astronomy, University of California, Irvine, California 92697*
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We present a Density Matrix Renormalization Group (DMRG) study of the ground-state properties of spin-1/2 frustrated $J_1 - J_3$ Heisenberg n_l-leg ladders (with n_l up to 8). For strong frustration ($J_3/J_1 \simeq 0.5$), both even- and odd-leg ladders display a finite gap to spin excitations, which we argue remains finite in the two-dimensional limit. In this regime, on odd-leg ladders the ground state is spontaneously dimerized, in agreement with the Lieb-Schultz-Mattis prediction, while on even-leg ladders the dimer correlations decay exponentially. The magnitude of the dimer order parameter decreases as the number of legs increases, consistent with a two-dimensional spin-liquid ground state.

Despite many years of intense investigations, the existence of a homogeneous spin-liquid ground state for a spin-1/2 system on a two-dimensional square lattice remains controversial. This is mainly because there has been no definite evidence so far that a microscopic model could stabilize a homogeneous non-magnetic phase with one electron per unit cell. In fact, the known non-magnetic phases of spin-1/2 quantum antiferromagnets in one or two dimensions usually display a spontaneously broken translation symmetry related to spin-Peierls dimerization, as in the frustrated Heisenberg chain [1, 2] and ring exchange models, [3], or arising from a doubling of the ground-state unit cell, as in the Heisenberg two-leg ladder.[4]

For one-dimensional systems a rigorous result, the Lieb-Schultz-Mattis (LSM) theorem, [5] implies that a gapped non-magnetic phase is in general associated with a broken translation symmetry. This result can be also extended to spin-1/2 Heisenberg models defined on odd-leg ladder geometries.[6] There have been several recent attempts to generalize the LSM result to two dimensions [7, 8, 9]. Here it has been argued that the gapped phase is associated with a ground-state degeneracy. However, there are different opinions on whether this degeneracy necessarily implies a spontaneously broken translation symmetry (and thus the non-existence of a two-dimensional spin-liquid) or whether it is associated with a topological degeneracy of fractionalized spin-liquid phases [7, 10, 11, 12]. Recently, on the basis of a variational approach, Sorella *et al.*,[13] have proposed that a spin-liquid ground state can be stabilized in two-dimensions and yet satisfy the constraint imposed by the LSM theorem. In fact, within the formalism of projected BCS wave functions it is possible to construct a gapped state which displays spontaneous dimerization on any odd-leg ladder thus satisfying the LSM theorem, but with no dimerization for even-leg ladders. The two-dimensional thermodynamic limit is consistently reached for a large number of legs since the dimer order parameter on odd-leg ladders vanishes in this limit, thus leading to a homogeneous spin liquid. In this case, therefore, the ground-state degeneracy predicted by the generalizations of the LSM theorem [9] is not connected to a spontaneously broken translation symmetry but rather to a topological degeneracy of fractionalized resonating valence bond states.[12, 13]

In this paper, we examine n_l-leg frustrated Heisenberg ladders with Hamiltonian

$$\hat{H} = J_1 \sum_{\langle i,j \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_3 \sum_{\langle\langle i,j \rangle\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \quad . \tag{1}$$

Here $\hat{\mathbf{S}}_i$ are spin-1/2 operators on a square lattice, and $J_1, J_3 \geq 0$ are the nearest- and third-nearest neighbor antiferromagnetic couplings along the two coordinate axes. In the following, we use the numerical density matrix renormalization group (DMRG) [14] to study the ground state of this Hamiltonian on ladder systems with n_l legs of length L with open boundary conditions. In our calculations, we typically performed 15-20 sweeps of the lattice, keeping a maximum of $m \simeq 2000$ states and obtaining discarded weights smaller than $\sim 5 \times 10^{-7}$. Our plan is to carry out DMRG calculations for ladders with different number n_l of legs. Then, by extrapolating in the length L of the ladders and looking at the behavior of the odd-and even leg systems for modest value of n_l we seek to gain insight into the behavior of the two-dimensional system.

The classical ground state of the $J_1 - J_3$ Hamiltonian in two dimensions displays conventional Néel order for $J_3/J_1 \leq 0.25$. For $J_3/J_1 > 0.25$ the ground state has incommensurate antiferromagnetic order with a pitch vector depending on the frustration ratio, assuming the value $Q = (2\pi/3, 2\pi/3)$ at $J_3/J_1 = 0.5$, and approaching $Q = (\pi/2, \pi/2)$, corresponding to four decoupled Nèel lattices, for $J_3/J_1 \to \infty$. For the case of quantum spin-1/2, in two-dimensions, the ground state is expected to display long-range Néel order for $J_3/J_1 \to 0$, and numerical calculations on lattices up to 32 sites suggest that a non-magnetic ground state could be stabilized in the regime of strong frustration $J_3/J_1 \sim 0.5$.[15] This

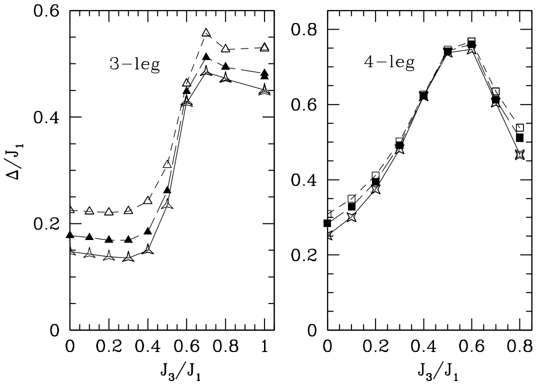

FIG. 1: Spin gap as a function of the ratio J_3/J_1. Left: 3-leg ladder for $N = 12$ (empty triangles), 16 (full triangles), and 20 (stars). Right: 4-leg ladder for $N = 10$ (empty squares), 12 (full squares), and 16 (stars).

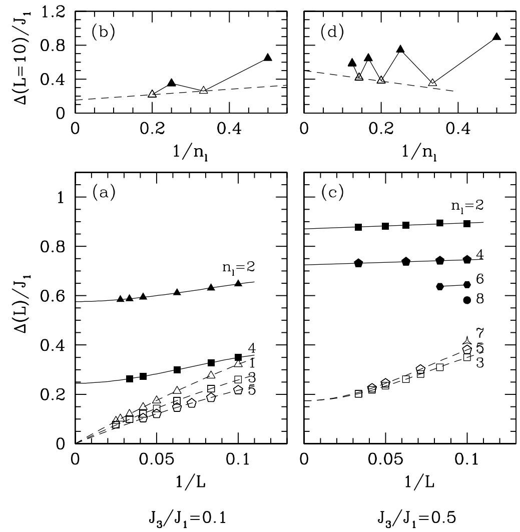

FIG. 2: Size scaling of the spin gap for $J_3/J_1 = 0.1$ [(a) and (b)], and $J_3/J_1 = 0.5$ [(c) and (d)]. (a) and (c): spin gap as a function of the length of the ladders, L, for different number of legs, n_l. (b) and (d): spin gap as a function of n_l, for $L = 10$. Empty (full) symbols correspond to odd- (even-) leg ladders. Lines are guides for the eye.

work also found signatures of dimerization for values of $J_3/J_1 \simeq 0.7$ in agreement with the predictions of series expansions.[16]

The effects of frustration on the antiferromagnetic correlations of the ground state can be investigated by studying the behavior of the spin-gap as a function of J_3/J_1. In fact, in a system with long-range spin correlations, spin excitations are necessarily gapless. Instead, if the energy cost of the lowest triplet excitation, Δ, remains finite in the thermodynamic limit the ground state has short-range spin-correlations. As shown in Fig. 1, for $n_l = 3$ and 4, the spin gap increases as the frustration ratio J_3/J_1 increases. This is seen for both the even- and the odd-leg ladder case. In particular, in the odd-leg case, which is gapless with power-law spin correlations in the pure Heisenberg limit,[17] the spin gap due to the finite length of the ladder remains almost constant for small values of J_3/J_1 but increases sharply for $J_3/J_1 \simeq 0.4$, suggesting a transition to a gapped non-magnetic phase. Alternatively, in the even-leg ladder case, a finite correlation length is expected for small J_3/J_1 and the spin-gap increases smoothly with J_3/J_1 as no magnetic transition is expected. In both cases, the spin gap reaches a maximum for intermediate values of J_3/J_1 where the effects of frustration are expected to be the strongest, then it decreases again for large J_3/J_1 when the limit of four decoupled Heisenberg lattices is eventually recovered.

The size scaling of the spin gap is shown in Fig. 2. For weak frustration, the spin gap extrapolates to zero for the odd-leg ladders, and to a constant, which decreases with n_l, for the even-leg ladders.[18] This is consistent with the gapless Nèel ordered phase expected in the two-dimensional limit. Instead, for $J_3/J_1 = 0.5$ the spin gap extrapolates to a constant as $L \to \infty$ for both the even- and the odd-ladders we have studied. The difference between the regime of low and high frustration is also seen from the dependence of the spin-gap on the number of legs for a fixed chain length L (see also Fig. 2-(b) and (d)). For low-frustration the spin-gap decreases with the number of legs both for even (full symbols) and odd (empty symbols) n_l. However, in the regime of high frustration it decreases with n_l only for even leg samples while it *increases* with the number of legs on odd-leg samples. This behavior is consistent with a two-dimensional phase which has exponentially decaying spin correlations.

The presence of a finite-gap in the excitation spectrum of the n_l-leg ladders has consequences in view of the LSM theorem. In fact, on odd-leg ladder systems it is possible to construct an excitation in the singlet sector with momentum $(\pi, 0)$ which becomes degenerate with the ground state in the thermodynamic limit.[5] This implies either a gapless spectrum or, in the presence of a finite gap, a two-fold degenerate ground state with a doubling of the unit cell and a spontaneously broken translation symmetry. In the one dimensional model this is known to be realized through spin-Peierls dimerization.[1] Instead, the LSM result does not apply to even-leg ladders so that, in these geometries, both translationally invariant and dimerized ground states are in principle compatible with a finite triplet gap.

The occurrence of spin-Peierls dimerization can be studied by calculating the response of the system to a nearest-neighbor spin-spin operator which breaks the translation symmetry along the chains with momentum $Q = (\pi, 0)$

$$\hat{O} = \sum_r e^{iQ\cdot r} \hat{\mathbf{S}}_r \cdot \hat{\mathbf{S}}_{r+x} \ . \qquad (2)$$

Here $x = (1, 0)$ is a unit vector along the chain direction.

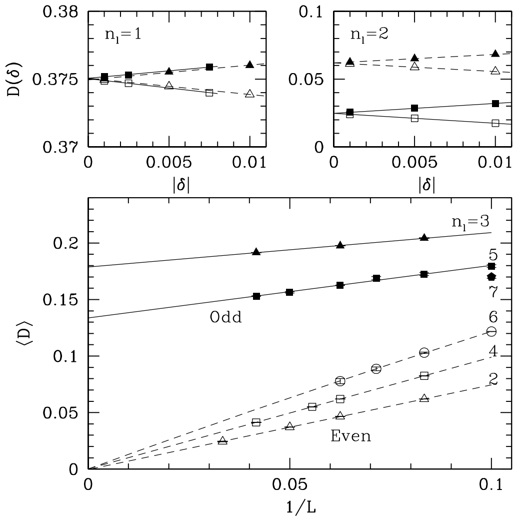

FIG. 3: Upper panels: $D(\delta)$ for $J_3/J_1 = 0.5$. Left: one dimensional (Majumdar-Gosh) chain for $N = 12$ (triangles), and 24 (squares). Right: 2-leg ladder for $N = 12$ (triangles), and 30 (squares). Full (empty) symbols correspond to $\delta < 0$ ($\delta > 0$). Lower panel: size-scaling of the dimer order parameter, $D(\delta \to 0)$, as a function of the length of the ladders, L, for different numbers of legs, n_l.

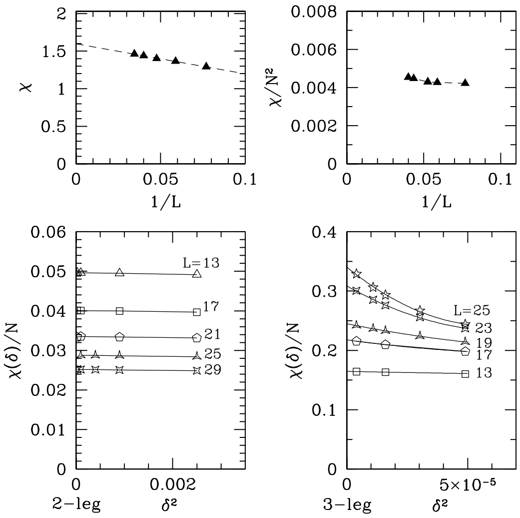

FIG. 4: Dimer susceptibilities for the 2-leg (left panels) and 3-leg (right panels) ladders. The lower panels show $\chi(\delta)/N$ *vs* δ for various lengths, and the top panels the size scaling of the extrapolated values, $\chi = \lim_{\delta\to 0}\chi(\delta)$ (see text). Note the different normalizations for the 2- and 3-leg cases in the upper panels. Lines are guides for the eye.

This can be done in general by adding to the Hamiltonian a term $\delta\hat{O}$ where δ is a (small) generalized field. The order parameter can be calculated as the limit for $\delta \to 0$ of the ground-state expectation value of $\hat{O}$ in presence of the field, $D = \lim_{\delta\to 0}\langle\hat{O}\rangle_\delta/N$, where $N = L \times n_l$ is the total number of sites. On periodic finite-size systems D vanishes in general by symmetry as it breaks the translational invariance and the symmetry under *site-centered* lattice reflections along the chain direction of the unperturbed Hamiltonian (1). However, on samples with an even length L and open boundary conditions, the dimer order parameter (2) will be in general non-zero and can be calculated using the Hellmann-Feynman theorem as $D = de(\delta)/d\delta|_{\delta=0}$. Here $e(\delta)$ is the ground-state energy per site (in unit of J_1) in the presence of the perturbation. As a result, within the DMRG technique the dimer order parameter can be calculated with simple energy measurements by computing $e(\delta)$ for a few values of δ and then estimating numerically the limit $D = \lim_{\delta\to 0}(e(\delta) - e_0)/\delta$. This is illustrated in the upper panels of Fig. 3 for a single chain and a two-leg ladder at $J_3/J_1 = 0.5$. Here, as a consistency check, the dimer order parameter is estimated by calculating the limit for $\delta \to 0$ of $D(\delta) = (e(\delta) - e_0)/\delta$ both for positive (filled symbols) and negative (empty symbols) δ's. The two limits converging to the same value. In particular, for the one-dimensional chain at the exactly solvable point $J_3/J_1 = 0.5$ (Majumdar-Gosh model) the known size-independent result, $D = 0.375$, is recovered [1].

The size scaling of the dimer order parameter obtained with this procedure is shown in the same figure for ladders with different numbers of legs. This analysis reveals close similarities with the variational scenario of Ref. [13]. In fact, in the odd-leg ladder case the dimer order parameter extrapolates to a constant for infinite chain length, as required by the LSM theorem. Instead, in the even-leg cases, where the system is not constrained by the LSM theorem to dimerize, the dimer order parameter extrapolates to zero.

This conclusion is supported also by the calculation of dimer susceptibilities. These can be calculated within our numerical approach by considering ladders with odd length L. In these geometries the unperturbed Hamiltonian is reflection symmetric around the central column of sites, so that the order parameter D vanishes by symmetry for any finite-size cluster, and the ground-state energy has corrections proportional to δ^2. Therefore $e(\delta) \simeq e_0 - \chi\delta^2/2$, with χ the generalized susceptibility associated with the operator $\hat{O}$, namely, $\chi = 2\langle\psi_0|\hat{O}(E_0 - \hat{H})^{-1}\hat{O}|\psi_0\rangle/N$. If true long-range order in the dimer correlations exists in the thermodynamic ground state, the finite-size susceptibility will diverge as the system size increases. In particular, it can be shown that it is bounded from below by the system volume squared, $\chi \sim N^2$. [19] Thus susceptibilities are a sensitive tool for detecting the occurrence of long-range order. In analogy with the calculation of the order parameter, the susceptibility $\chi = -d^2e(\delta)/d\delta^2|_{\delta=0}$ can be calculated numerically from $\chi = \lim_{\delta\to 0}\chi(\delta) = -2(e(\delta) - e_0)/\delta^2$, as illustrated in the bottom panels of Fig. 4 for 2- and 3-leg ladders.

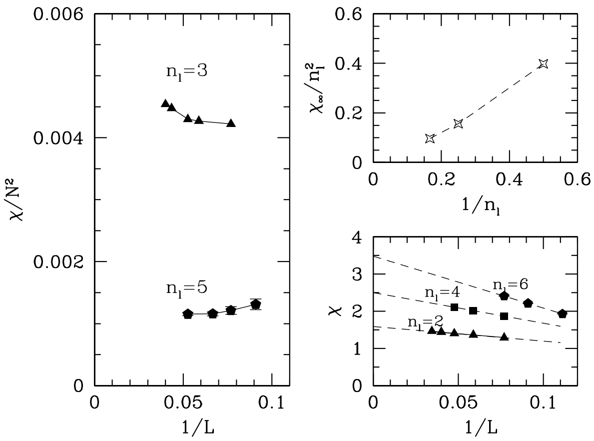

FIG. 5: Left: Size scaling of χ/N^2 for the 3- and 5-leg ladders as a function of the chain-length L. Right bottom: Size scaling of χ for the 2-, 4- and 6-leg ladders as a function of the chain-length L (bottom). Right top: Size scaling of the $L \to \infty$ extrapolated values of the even-leg ladder susceptibilities, χ_∞, as a function of the numbers of legs, n_l.

The behavior of the susceptibilities for the even- and odd-leg ladders is remarkably different (Fig. 4). In particular, χ/N decreases with the linear size L in the even-leg ladder case, and it increases with L in the odd-leg ladder case. The susceptibilities for the odd-leg ladders appear to diverge as N^2, as required for true long-range dimer order. In contrast, for the even-leg ladders the susceptibilities are bounded, indicating short-range dimer correlations with a finite correlation length.

In order for the two-dimensional limit to exist, the ground-state correlations for even and odd-leg ladders must converge in the limit of a large number of legs. This is the case, for instance, in the limit of small frustration of this model, where the spin correlations decay exponentially for even n_l and with a power-law for odd n_l. Here the two-dimensional limit is reached as the correlation length for the even-leg ladders diverges exponentially with n_l leading to long-range antiferromagnetic order in two dimensions. [17, 18] As we have shown, in the regime of strong frustration, the dimer-correlations are short-ranged on even-leg ladders while a finite-dimer order parameter is observed on odd-length ladders. However, as the number of chains n_l is increased, the odd-leg ladder dimer order parameter decreases (Fig. 3), and the divergence of the dimer susceptibility becomes weaker (see left panel of Fig. 5). On the other hand, the infinite-L dimer susceptibility, χ_∞, on even-leg ladders does not appear to diverge as the square of the number of chains, n_l^2, (see right-panels of Fig. 5) as one would expect in presence of long-range dimer order in two dimensions. Thus, a ground-state with no spontaneous broken translation symmetry in the two-dimensional limit appears as a plausible interpretation of our results.

In conclusion, we have shown that a spin-gapped ground state with short-range antiferromagnetic correlations is stabilized by frustration on the spin-1/2 J_1−J_3 model at $J_3/J_1 = 0.5$ on ladders with $n_l = 1$ to 8 legs. The behavior of the spin gap by increasing the number of legs is consistent with a non-magnetic ground state in the two-dimensional limit. On odd-leg ladders we find a finite dimer order parameter associated with a spontaneously broken translation symmetry. However, as the number of legs increases $n_l = 1, 3, 5, 7$ the size of the order parameter decreases and the divergence of the associated susceptibility becomes weaker. These results suggests that in the two-dimensional limit the dimer order parameter vanishes. Although the numerical data we have presented here was for $J_3/J_1 = 0.5$, we find similar results for other values of J_3/J_1 near 0.5 and believe that for a range of J_3/J_1 values this model exhibits a non-magnetic ground state in two dimensions. Our results are consistent with a recently proposed scenario [13] where the odd-leg dimer order vanishes for infinite number of legs leading to a homogeneous spin-liquid in two dimensions.

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